Derivation of Ohm's Law in a Deterministic Mechanical Model

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Abstract

We study the Lorentz gas in small external electric and magnetic fields, $\mathbf{E}$ and $\mathbf{B}$, with the particle kinetic energy held fixed by a Gaussian "thermostat" (a modification of a model of Moran and Hoover.) Here we prove rigorously that : (1) Starting from any smooth initial density, a unique stationary, ergodic measure (whose support is fractal) is approached for times $t \to \infty$. (2) The steady-state electric current, $\mathbf{J}(\mathbf{B}, \mathbf{E})$, is given by a Kawasaki formula and the entropy production $\mathbf{J} \cdot \mathbf{E}/T$, with T the "temperature," is equal to both the asymptotic decay rate of the Gibbs entropy and minus the sum of the Lyapunov exponents. (3) The Einstein relation and Kubo formulas hold, i.e. $\mathbf{J}(\mathbf{B}, \mathbf{E}) = \sigma(\mathbf{B}) \cdot \mathbf{E}+$ higher order terms, with the diffusion matrix $\mathbf{D}(\mathbf{B})$ at $\mathbf{E} = 0$ given by $k_B T$ times the symmetric part $\tilde{\sigma}(\mathbf{B})$ of the conductivity matrix.

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We consider the Lorentz model of a metallic conductor given by a classical point-particle or a non-interacting gas of such particles ("electrons") moving in a periodic array of fixed, hard, convex scatterers ("ions"). Here we study the validity of *Ohm's law* in the presence of applied fields. At present, no general statistical mechanical theory can predict which microscopic dynamics will yield such transport laws, and their derivation has been referred to by Peierls as one of the outstanding unsolved problems of modern physics [1]. In addition to this fundamental interest, our work may also be of relevance to some beautiful experimental systems constructed recently by microfabrication—the so-called "antidots"—which are lattice structures with periodicities of order 10^2 nm [2]. The experimental observation of magnetoresistance in these systems, with Fermi wavelength smaller than the superlattice spacing, has been interpreted with reasonable success in terms of classical dynamics [2].

The Lorentz model, also known as the dispersed billiard, possesses very strong hyperbolic properties which allow the diffusive Brownian motion of (undriven) test particles to be rigorously established in a long length- and time-scale limit [3]. This requires that the scatterer configuration have *finite horizon*, so that any particle travels only a uniformly bounded time freely between collisions. (When there is infinite horizon—as is typically the case for the antidots [1]—the diffusion is expected to be anomalous with the mean-square displacement growing like $t \log t$ [4].) However, under the influence of an applied electric field, the particles in this model accelerate without any limiting velocity, because there is no dissipative mechanism to absorb the energy put in as work by the electric field. The actual drift appears to be sublinear, with the net displacement in the direction of the field apparently growing like $t^{2/3}$. This was noted by Moran and Hoover [5], who proposed and studied numerically a modification of the Lorentz gas which incorporates a frictional term designed to model the interaction of the test particle with a "heat bath". The friction coefficient is chosen according to Gauss' "principle of least constraint" [6], so that the kinetic energy of the particle is held at a fixed constant value. This is a simple example of a new method in non-equilibrium molecular dynamics (NEMD) which has been developed in the past decade by Evans, Hoover, Morriss, Nosé and others [7].

To state precisely the model, the motion between collisions is governed by the set of first-order equations

$$\dot{\mathbf{q}} = \mathbf{p}/m \tag{1}$$

$$\dot{\mathbf{p}} = \mathbf{E} + \mathbf{p}\times\mathbf{B} - \zeta \cdot \mathbf{p} \tag{2}$$

$\mathbf{q} = (q_1, ..., q_d)$ are the Cartesian coordinates of the particle, $\mathbf{p} = (p_1, ..., p_d)$ are the corresponding momenta, and we have added to the Moran-Hoover model a Lorentz force produced by an external magnetic field. The "friction coefficient" ζ is chosen as

$$\zeta = \mathbf{E} \cdot (\mathbf{p}/m)/(p^2/m), \tag{3}$$

so that kinetic energy is fixed. Although our work can be generalized to $d > 2$, we only discuss here $d = 2$. The reduced phase space, at each fixed value of the particle speed v, has coordinates $X = (q_1, q_2, \theta)$, where θ is the angle of the particle velocity vector with respect to the 1-direction. It is easy to verify that the divergence of the dynamical velocity vector $\dot{X}$ is $-\zeta$, so that the Liouville measure $d\mu_0 = d\mathbf{q}d\theta$ is not preserved when $E \neq 0$. On the other hand, observe that Eqs.(1)-(3) define a flow on the phase-space, running backward as well as forward, and reversible, i.e. starting from an initial phase point $X(0)$ we get $X(t)$ for all t and if one reverses velocities and magnetic fields at $t = \tau$ then $X(t + 2\tau)$ is just $X(0)$ with velocities reversed.

It should be emphasized that for a correct application of the general NEMD method one should properly consider an N-particle system with N large. In that situation, holding the total kinetic energy $K = \frac{1}{2}\sum_{i=1}^{N} m_i\dot{\mathbf{q}}_i^2$ fixed should arguably be equivalent to holding the temperature fixed, with the identification $K = N \cdot d \cdot k_B T/2$. Eqs. (1) and (2) would then hold for each $(\mathbf{q}_i, \mathbf{p}_i)$ with $\zeta = \mathbf{E} \cdot \sum_i \mathbf{v}_i/2K$. It is easy to check that

$$\nabla_X \cdot \dot{X} = -\mathbf{E} \cdot \mathbf{J}(X)/k_B T \tag{4}$$

follows, with $\mathbf{J}(X) = \sum_{i=1}^{N} \mathbf{v}_i \sim$ of order$N$ and with a correction of relative order unity neglected. Remarkably, the expression $\mathbf{E} \cdot \mathbf{J}(X)$ has the form of "force" times (microscopic) "flux," which is identical to the form of entropy production in phenomenological thermodynamics. It is this crucial relation that, in our opinion, is the important feature of Gaussian dynamics which accounts for its successful representation of the steady state. In our simple example with $N = 1$ the identification of "temperature"— according to the above prescription— as the non-fluctuating kinetic energy of a single particle lacks physical justification and, also, fails to satisfy the crucial Eq.(4). Therefore, we here define "temperature" as twice that value, i.e. $k_B T = 1/\beta = p^2/m$, just so that the equation $\nabla_X \cdot \dot{X} = -\mathbf{E} \cdot \mathbf{v}/k_B T$ analogous to Eq.(4) still holds.

We now present our results for the case $N = 1$, using, however, a slightly different form than that in which they are rigorously obtained [8]. For the mathematical proofs we must consider a discrete-time description of the system in which time is counted by number of successive collisions of the particle with scatterers, a so-called *special representation* of the flow. It is only in the discrete-time representation that we can presently obtain the good decay of correlations for Eqs.(6) or (8) below, for example.

First, we show that starting from any probability distribution $f_0(X)dX$ on the three dimensional phase space, a unique ergodic measure μ^+ is obtained by evolving forward in time. This result is obtained at least when E and B are sufficiently small and the condition of finite-horizon holds for zero field. Furthermore, there is a very simple integral formula for the average $\langle\phi\rangle^+$ of any continuous function $\phi(X)$ in this stationary state. For a formal derivation, note that the average of ϕ at time t—starting from an initial constant ensemble density, $f_0(X) = C$—is given by a simple calculation to be

$$\langle\phi\rangle_t = \langle\phi\rangle_0 + \beta\mathbf{E}\cdot \int_0^t \langle\mathbf{v}\phi(X_{\mathbf{B},\mathbf{E}}(s))\rangle_0 ds \tag{5}$$

where $\langle\phi\rangle_t$ is the average with respect to the ensemble density at time t. For clarity the $\mathbf{B}, \mathbf{E}$-dependence of the phase trajectory $X(t)$ under the dynamics is explicitly indicated. Under the stated assumptions, we show that $\langle\phi\rangle_t$ converges to $\langle\phi\rangle^+$ as $t \to +\infty$, and, furthermore, the integrand on the right side of (5) has sufficiently good decay so that the limit $t \to +\infty$ may be taken there. We obtain finally

$$\langle \phi \rangle^+ = \langle \phi \rangle_0 + \beta \mathbf{E} \cdot \int_0^\infty \langle \mathbf{v} \phi(X_{\mathbf{B},\mathbf{E}}(t)) \rangle_0 \, dt. \tag{6}$$

While such expressions for steady-state measures have been known for a long time [9], they are generally purely formal since the convergence of the integral is not known.

¿From Eq.(6) with $\phi = \mathbf{v}$, one obtains a formula for the exact current-response as a nonlinear function of field:

$$\mathbf{J}(\mathbf{B}, \mathbf{E}) \equiv \langle \mathbf{v} \rangle^+ = \beta \mathbf{E} \cdot \int_0^\infty \langle \mathbf{v} \mathbf{v}_{\mathbf{B},\mathbf{E}}(t) \rangle_0 \; dt. \tag{7}$$

This is an example of a so-called *Kawasaki formula* for the nonlinear response [10] and it describes a variety of phenomena, including the usual *Hall effect* of transverse electric currents in a magnetic field. The response to linear order in the field is then given by

$$\langle \phi \rangle^+ = \langle \phi \rangle_0 + \beta \mathbf{E} \cdot \int_0^\infty \langle \mathbf{v} \phi(X_{\mathbf{B},\mathbf{0}}(t)) \rangle_0 \; dt + \text{higher order terms in } E. \tag{8}$$

To prove this rigorously correct we establish a bound on the decay in t of $\langle \mathbf{v} \phi(X_{\mathbf{B},\mathbf{E}}(t)) \rangle_0$ uniform in E, which allows standard convergence theorems to be applied to show that the remainder term is really of higher order in E. This is not just a fine point of rigor but is exactly where dynamical properties enter in the derivation of the transport law. From Eq.(8) one obtains directly *Ohm's law* $\mathbf{J}(\mathbf{B}, \mathbf{E}) = \sigma(\mathbf{B}) \cdot \mathbf{E} +$ higher order, with the conductivity tensor $\sigma(B)$ given by

$$\sigma(\mathbf{B}) = \beta \int_0^\infty \langle \mathbf{v} \mathbf{v}_{\mathbf{B},\mathbf{0}}(t) \rangle_0 \, dt, \tag{9}$$

a usual *Kubo formula* for the conductivity [11]. The formal linear response calculations given above can be made quite generally, and suggest that the integrable decay of the Green-Kubo formula (uniformly in the mechanical or thermodynamical force) is the necessary and sufficient condition for validity of the standard linear transport law [12]. Since the diffusion matrix $\mathbf{D}(\mathbf{B})$ describing the mean-square deviation of test-particles from their expected motion in zero electric field can be shown to be given also by a Green-Kubo formula $\mathbf{D}(\mathbf{B}) = \frac{1}{2} \int_{-\infty}^{+\infty} \langle \mathbf{v} \mathbf{v}_{\mathbf{B},\mathbf{0}}(t) \rangle_0 \, dt$ (generalizing that for $\mathbf{B} = \mathbf{0}$ in [3]), we obtain immediately also a (generalized) *Einstein relation*

$$\tilde{\sigma}(\mathbf{B}) = \beta \cdot \mathbf{D}(\mathbf{B}), \tag{10}$$

where $\tilde{\sigma}$ denotes the symmetric part of σ. Note that the β appearing here comes directly from the formal definition of T in (4): it all hangs together.

To prove the above results we show that the dynamical system may be very well approximated by a certain stochastic Markov chain. This approximation is obtained by means of a so-called *Markov sieve*[13]. The method of proof can be viewed as a realization at a sophisticated mathematical level of the "stochastization" of a dynamical particle system by a "coarse-graining" of the phase-space. Rather than follow the detailed trajectory in the phase space, one may consider just the transition of the phase point from cell to cell of the coarse-graining partition under successive time-steps.

In the context of the Gaussian method there is a very remarkable relation, noted in [5], which arises between the time-derivative of the Gibbs entropy, the Lyapunov exponents of the dynamics, and physical entropy production; see also [7]. We can rigorously establish this relation (using the definition of temperature which comes from Eq.(4)), as we briefly indicate here. First, with the usual definition of Gibbs entropy, $S(t) = -k_B \int f_t(X) \log f_t(X)\ dX$, where f_t is the ensemble density at time t. It is a simple calculation that $\dot{S}(t) = k_B \int\ f_t(X)(\nabla_X \cdot \dot{X})\ dX = -k_B\langle\zeta\rangle_t$. Using Eq.(4) we can therefore infer that

$$-\dot{S}(t) \to k_B\ \langle\zeta\rangle^+ = \mathbf{J}\cdot\mathbf{E}/T, \tag{11}$$

as $t \to +\infty$, where the right side is just the entropy production due to Ohmic dissipation. This can be understood if one imagines that the Gaussian dynamics model the effect of reservoir elements on the particle system, for which the *total* system, reservoir+particles, obeys the Liouville theorem. Hence, the decrease of particle entropy corresponds to the increase of reservoir entropy, and the latter represents the physical entropy production. This result gives some support, in fact, to the interpretation of Gaussian dynamics as an adequate model for the effects of a heat bath (at least, as discussed above, for large N.)

On the other hand, the divergence of the dynamical vector field can also be related to the rate of change of Liouville volume in the phase space. It is heuristically obvious that the steady-state expected rate of volume contraction should be equal to the sum of the stable and unstable Lyapunov exponents $\lambda^s_{\mathbf{B},\mathbf{E}} < 0$ and $\lambda^u_{\mathbf{B},\mathbf{E}} > 0$ of the flow, defined and almost surely constant with respect to the ergodic measure μ^+. In our case this can be proved, and we obtain the relation

$$-\dot{S}(t) \to k_B(\lambda^s_{\mathbf{B},\mathbf{E}} + \lambda^u_{\mathbf{B},\mathbf{E}}) \tag{12}$$

for $t \to +\infty$. Putting together the two expressions for the asymptotic decay of Gibbs entropy we obtain finally the relation

$$\mathbf{E}\cdot\mathbf{J}/T = -k_B(\lambda^s_{\mathbf{B},\mathbf{E}} + \lambda^u_{\mathbf{B},\mathbf{E}}), \tag{13}$$

which directly relates entropy-production and Lyapunov exponents. In the limit $E \to 0$, this yields also a relation between diffusion coefficient and Lyapunov exponents of the Gaussian dynamics with respect to μ^+: $\hat{\mathbf{e}}\cdot\mathbf{D}(\mathbf{B})\cdot\hat{\mathbf{e}} = \lim_{E\to 0} -k_B T^2(\lambda^s_{\mathbf{B},\mathbf{E}} + \lambda^u_{\mathbf{B},\mathbf{E}})/E^2$ (where $\hat{\mathbf{e}}$ is the unit vector in the direction of $\mathbf{E}$). Such relations are believed to also extend to other more complicated many-particle situations [14].

Since it is known that $\mathbf{D} > \mathbf{0}$, it follows from the relation like Eq.(11) that the Gibbs entropy starting from an initially smooth distribution has an asymptotically constant rate of decrease. Therefore, one expects S in the stationary state μ^+ to be $-\infty$, and, in particular, that μ^+ will be singular with respect to Liouville measure μ_0 i.e. it will have a support with fractal dimension less than three, which is the dimension of the energy surface [5, 7]. In fact, we can show, in agreement with the numerical results [5, 15], that this is indeed the case. More precisely, we can show that the *Young's formula* for the Hausdorff dimension (HD) of the measure is valid [16](see also [17]). This here states that $HD(\mu^+) = 1 + h[(\lambda^u)^{-1} - (\lambda^s)^{-1}]$ in which $h = \lambda^u$ is the dynamical Kolmogorov-Sinai entropy of the flow defined by Eqs.(1)-(3). (The equality $h = \lambda^u$ is called Pesin's formula [17]). Using the relationship between Lyapunov exponents and transport coefficients, it then follows that for small E

$$HD(\mu^+_{\mathbf{B},\mathbf{E}}) = 3 - \frac{\mathbf{E} \cdot \sigma(\mathbf{B}) \cdot \mathbf{E}/T}{k_B \cdot h_{\mathbf{B},\mathbf{0}}} + \text{higher order corrections.} \tag{14}$$

In particular, it follows that $HD(\mu^+) < 3$ when E is small but finite.

Although no rigorous or reliable numerical results are available for many-particle systems, we do *not* expect that this "dimensional reduction" will persist in an extensive sense at least in those systems where the particles are in a state of *local equilibrium.* That is, in the appropriate "hydrodynamic limit" for such systems in which particle number and volume both go to infinity, we expect the ratio of the Hausdorff dimension and phase space dimension to go to unity, just because the system is then composed of small "local equilibrium regions" in which the distribution is (nearly) given by an absolutely continuous Gibbs measure. It should be noted anyway that the phenomenon of "dimensional reduction" is a property just of the representation of thermal reservoirs by Gaussian dynamics, and can be proved *not* to occur, for example, with suitable stochastic representation of heat baths [18]. On the other hand, we would not be surprised if the "dimensional reduction" per degree of freedom persists in the infinite volume limit—for the stationary measures of Gaussian-type dynamics—in those situations where local equilibrium breaks down, e.g. where the velocity distribution is not close to a Maxwellian. This would be the case for current-carrying electrical conductors. For some further discussion, see [19]. The stationary measures μ^+ we construct here, although singular with respect to Liouville measure, have the property that they are smooth in the unstable directions of the flow. The property is clearly evidenced in the computer simulations of the density found from the time sampling of phase-points, which shows a concentration along the unstable manifolds: see [5]. This property implies, in particular, the smoothness of the reduced measures for the system, e.g. the positional density or the probability density of the x-component of the velocity. In fact, the measure μ^+ is just a particular case of the so called Sinai-Ruelle-Bowen-measures for our hyperbolic system, constructed previously for smooth systems (e.g. see [17]).

All of the formal arguments given above extend to the general N-particle model and lead to the reasonably expected results, so that we expect our theorems hold also in the general case. Unfortunately, because of lack of strict hyperbolicity for the many-particle case, we cannot rigorously study by our method the small-field perturbation in those models. On the other hand, we have for this model a *rigorous* proof of the validity of linear response theory—despite the fact that the dynamics of individual trajectories are sensitively dependent upon the presence or absence of the field. Therefore, our work can be regarded as a counterexample to some of the objections raised by van Kampen against linear response theory [20]. For a fuller discussion of this point we refer to our longer work [8], in which also the proofs of the main propositions announced here are given.

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